

Braggoriton–Excitation in Photonic Crystal Infiltrated with Polarizable Medium

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Light propagation in a photonic crystal infiltrated with polarizable molecules is considered. We demonstrate that the interplay between the spatial dispersion caused by Bragg diffraction and polaritonic frequency dispersion gives rise to novel propagating excitations, or *braggoritons*, with intragap frequencies. We derive the braggoriton dispersion relation and show that it is governed by two parameters, namely, the strength of light-matter interaction and detuning between the Bragg frequency and that of the infiltrated molecules. We also study defect-induced states when the photonic band gap is divided into two subgaps by the braggoritonic branches and find that each defect creates *two* intragap localized states inside *each* subgap.

I. Introduction

Photonic crystals and in particular photonic band gap (PBG) materials^{1,2} have recently attracted much attention^{3,4} due to their rich physics and possible applications. In these systems the dielectric function is periodically modulated and, as a result, their optical properties are dominated by light diffraction effects. When Bragg diffraction conditions are met then light scattering is very strong, so that within certain frequency intervals near the resonances light propagation is inhibited.

Since the subject of photonic crystals was introduced,^{1,2} one of the main goals of photonic band-structure calculations was to engineer structures with a *complete* band gap, *i.e.* with no propagating solutions of Maxwell's equations within a certain *forbidden gap*. The pursuit of this goal has generated a stream of studies that are too numerous to be cited here; early works are reviewed in Refs. 3, 4. Here we only mention that a complete band gap in two dimensions (2D) was theoretically predicted^{5,6} and experimentally demonstrated⁵ for an array of dielectric rods. In the quest for a structure having a complete PBG in three dimensions (3D), the diamond lattice was shown⁷ to be more promising than a simple face centered cubic (fcc) lattice^{7,8}.

The frequency gap in the photonic spectrum sets a stage for a number of physical effects. The prime effect, namely the inhibition of spontaneous emission for an emitter with transition frequency within the gap, was already suggested in the pioneering works.^{1,9,10} Furthermore, since light cannot leave the emitting atom, a coupled atom-field in-gap state is formed, in which the atomic level is “dressed” by its own exponentially localized radiation field.^{9,11} It was also demonstrated that although a single photon cannot propagate inside the gap, nevertheless a non-linear medium embedded inside the photonic crystal gives rise to multi-photon bound states¹², or gap solitons¹³ that result in self-induced transparency. Yet another consequence of PBG is the modification of cooperative emission with frequency close to the band edge. In particular PBG was shown to

change the rate of superradiant emission from an ensemble of emitters.^{10,14} Lastly, PBG structures facilitate strong Anderson localization of photons¹⁵ because the sharp density of states within the gap spectral range necessitates a reinterpretation of the Ioffe-Regel criterion.²

PBG structures with a defect constitute a separate area of study initiated by the classical works in Refs. 5, 16. These structures are important since the defects cause localized intragap states. For these states, the PBG sample acts as a resonator with a very high quality factor. This property was recently used for designing a low-threshold PBG defect-mode laser.¹⁷

Another class of materials with a forbidden gap for light propagation are spatially homogeneous, but frequency-dispersive media. The energy gap in these systems has a polaritonic origin, *i.e.* it is formed due to the interaction of light with the medium polarization.¹⁸ This energy gap can be viewed as the result of anticrossing between the photonic and excitonic dispersion relation branches. Some non-trivial manifestations of the polaritonic gap were recently explored in Refs. 19, 20. In these papers a general model of two-level systems interacting with elementary electromagnetic excitations with a gap in the spectrum was solved by means of the Bethe ansatz technique. Within this model a very rich excitation spectrum was found,^{19,20} consisting of ordinary solitons, single-particle impurity bound states and massive pairs of confined gap excitations and their bound complexes — dissipationless quantum gap solitons.

Most of the available photonic crystals nowadays however have *incomplete* PBGs; this means that light propagation is forbidden only along certain directions inside the crystal. A prominent example are opals, representing self-assembled monodispersed silica balls²¹ arranged in a fcc type lattice. Although opals have only incomplete PBG, the voids between the balls can be infiltrated by various media, which brings about non-trivial physics. In particular, the medium may contain polarizable molecules. Infiltrated opal with polarizable molecules combines therefore polaritonic and Bragg-diffractive properties. Obviously, both effects coexist in-

dependently when the Bragg ($\omega = \omega_B$) and polaritonic ($\omega = \omega_T$) resonances are well separated in frequency. A completely different situation occurs when $\omega_B \approx \omega_T$. This may be easily achieved in infiltrated opals that gives rise to a peculiar *interplay* between various frequency dispersions. This interplay is the subject of the present paper.

Our most important finding pertains to the case when the polaritonic gap of the polarized molecules infiltrating the opal lies within the opal PBG. We demonstrate that such an overlap gives rise to novel massive *propagating* excitations having frequencies inside the Bragg gap, that we dubbed here *braggoritons*. In other words, the Bragg gap *splits* into two sub-gaps, so that the braggoritonic branches are isolated from the rest of the spectrum. We found that the braggoriton dispersion relation is very sensitive to the frequency detuning between ω_B and ω_T and to the relative width of the polaritonic gap (or, alternatively Rabi frequency) and the Bragg gap.

The principal assumption we adopt here is that the Bragg gap, $\Delta\omega_B$, is narrow compared to ω_B ; this is actually the case in opals. The small value of $\Delta\omega_B/\omega_B (\ll 1)$ enables us then to obtain analytical results. In addition we also study the phase slip related intragap defect states for $\omega_B \approx \omega_T$. In the absence of polaritonic effect, the underlying physics of the defect-induced intragap states was already discussed in the original PBG paper¹. An analogy was drawn between a defect state and a localized mode in a distributed feedback resonator, that originates from a phase slip. We extend this picture to incorporate polarizable medium and show that when the Bragg gap splits into two sub-gaps, then an existing phase slip gives rise to *two* localized states with frequencies within *each* of the sub-gaps.

Our paper is organized as follows: In order to introduce the notations, we separately review in Sec. II the derivation of the PBG and polaritonic spectra using the second quantization representation. In Sec. III we consider the combined Hamiltonian in the second quantization representation and diagonalize it by a unitary transformation. This yields the dispersion relations for the two excitations outside the gap, or Bloch-like waves, and the two intragap branches, or braggoritons. The properties of these novel excitations are analyzed in Sec. IV. We use them in Sec. V to determine the intragap frequencies of the defect-induced localized states. Concluding remarks are presented in Sec. VI.

II. Second quantized PBG and polaritonic Hamiltonians

The Hamiltonian \mathcal{H} of the system under study is the sum of three terms

$$\mathcal{H} = \mathcal{H}_{\text{ph}} + \mathcal{H}_{\text{m}} + \mathcal{H}_{\text{m-ph}}. \quad (1)$$

The first term, \mathcal{H}_{ph} , describes the photons in a photonic crystal. The second term, \mathcal{H}_{m} , is the Hamiltonian of the polarizable medium; $\mathcal{H}_{\text{m-ph}}$ describes the photon-medium coupling. In this Section we review two limiting cases: (i) no polarizable medium ($\mathcal{H}_{\text{m}} \equiv 0$), and (ii) no modulation of the dielectric constant.

A. Incomplete PBG

The general form of the Hamiltonian \mathcal{H}_{ph} is

$$\mathcal{H}_{\text{ph}} = \frac{1}{8\pi} \int d\mathbf{r} [\varepsilon(\mathbf{r}) \mathbf{E}^2 + \mathbf{H}^2], \quad (2)$$

where \mathbf{E} and \mathbf{H} are respectively the electric and magnetic fields. For a constant dielectric function, $\varepsilon(\mathbf{r}) \equiv \varepsilon_0$, the second quantized form²² of the Hamiltonian (2) reduces to a sum over oscillators representing plane waves with frequencies $\omega_k = ck/\sqrt{\varepsilon_0}$, where k is the wave vector. Modulation of $\varepsilon(\mathbf{r})$ causes light diffraction, so that the plane wave solutions are no longer the correct eigenfunctions of the Hamiltonian (2). Below we consider a photonic crystal with an incomplete PBG along the z axis. This situation can be approximated by a one-dimensional modulation of $\varepsilon(\mathbf{r})$ along the z direction. If the Bragg gap is relatively narrow as assumed above, then it may be sufficient to consider only the first harmonics in $\varepsilon(z)$:

$$\varepsilon(z) = \varepsilon_0 + \delta\varepsilon \cos(\sigma z + \phi). \quad (3)$$

Here $\delta\varepsilon (\ll \varepsilon_0)$ is the modulation amplitude, $\sigma = 2\pi/d$, where d is the modulation period and ϕ is the dielectric modulation phase. We assume for simplicity that the electromagnetic field propagates along the z -direction and is homogeneous in the xy plane. In this case light polarization is irrelevant. Generalization to arbitrary propagation direction is straightforward. The Fourier components of $\varepsilon(z)$ in (3) couple the original photon oscillators with momenta k and $k \pm \sigma$. These coupled oscillators form an infinite series that is constructed by successive addition (subtraction) of σ . However, if $\delta\varepsilon \ll \varepsilon_0$ and the wavevectors domain is restricted to the vicinity of the first Bragg resonance at $k \approx \sigma/2$, then the Hamiltonian (2) can be truncated. In this case only the coupling to the near-resonance backscattered photons with momenta $(\sigma - k) \approx \sigma/2$ must be retained, so that the Hamiltonian (1) takes the form

$$\begin{aligned} \mathcal{H}_{\text{ph}} = & \sum_q \{ \omega(q) \hat{a}_{\rightarrow}^{\dagger}(q) \hat{a}_{\rightarrow}(q) + \omega(-q) \hat{a}_{\leftarrow}^{\dagger}(-q) \hat{a}_{\leftarrow}(-q) \\ & + \Omega_B [e^{i\phi} \hat{a}_{\rightarrow}^{\dagger}(q) \hat{a}_{\leftarrow}(-q) + e^{-i\phi} \hat{a}_{\leftarrow}^{\dagger}(-q) \hat{a}_{\rightarrow}(q)] \}. \end{aligned} \quad (4)$$

Here, we introduced the notations: $q = k - \sigma/2$, $\hat{a}_{\rightarrow}(q) = \hat{a}_k$ and $\hat{a}_{\leftarrow}(-q) = \hat{a}_{k-\sigma}$ for $k \approx \sigma/2$, where \hat{a}_k is the usual photon annihilation operator. In the notations introduced in (4), the frequencies of the photonic branches are given by:

$$\omega(q) = \frac{c(q + \sigma/2)}{\sqrt{\varepsilon_0}} = \omega_B \left(1 + \frac{2q}{\sigma} \right), \quad (5)$$

where $\omega_B = c\sigma/(2\sqrt{\varepsilon_0})$ is the Bragg frequency. We define the coupling constant, Ω_B , as the half-width of the Bragg gap, *i.e.* $\Omega_B = \frac{1}{2}\Delta\omega_B$. It can be shown that Ω_B is related to the amplitude of the dielectric function modulation: $\Omega_B = \omega_B \delta\varepsilon/(2\varepsilon_0)$. The summation in Eq. (4) is performed over the k domain $|q| \ll \sigma/2$.

It is straightforward to diagonalize the Hamiltonian in Eq. (4) with the use of the following unitary transformation

$$\begin{aligned} \hat{a}_\rightarrow(q) &= \cos\theta \hat{\beta}_1(q) + \sin\theta e^{i\phi} \hat{\beta}_2(q), \\ \hat{a}_\leftarrow(-q) &= -\sin\theta e^{-i\phi} \hat{\beta}_1(q) + \cos\theta \hat{\beta}_2(q), \end{aligned} \quad (6)$$

where

$$\cos 2\theta = \frac{\omega(q) - \omega(-q)}{\sqrt{[\omega(q) - \omega(-q)]^2 + 4\Omega_B^2}}. \quad (7)$$

The new operators \hat{B}_1 and \hat{B}_2 describe the creation (annihilation) of pairs of Bloch waves, that consist of forward and backscattered photons near the Bragg frequency. The diagonalized Hamiltonian (4) takes the form

$$\mathcal{H}_{\text{ph}} = \sum_q \omega_B^{(1)}(q) \hat{\beta}_1^+(q) \hat{\beta}_1(q) + \omega_B^{(2)}(q) \hat{\beta}_2^+(q) \hat{\beta}_2(q), \quad (8)$$

where the dispersion relations of the two photonic branches are given by:

$$\begin{aligned} \omega_B^{(1,2)}(q) &= \\ \frac{1}{2} \left[\omega(q) + \omega(-q) \pm \sqrt{(\omega(q) - \omega(-q))^2 + 4\Omega_B^2} \right] &= \\ \omega_B \pm \sqrt{\left(\frac{2\omega_B}{\sigma} \right)^2 q^2 + \Omega_B^2}. \end{aligned} \quad (9)$$

As mentioned above, the width of the PBG from Eq. (9) is $2\Omega_B$.

B. Polarizable medium

The Hamiltonians \mathcal{H}_m of polarizable medium and $\mathcal{H}_{m\text{-ph}}$ of light-polarization interaction in Eq. (1) can be written in the second quantization form as:

$$\begin{aligned} \mathcal{H}_m + \mathcal{H}_{m\text{-ph}} &= \omega_T \sum_k \hat{b}_k^+ \hat{b}_k \\ &+ \Omega_P \sum_k \left[\hat{b}_k^+ \hat{a}_k + \hat{a}_k^+ \hat{b}_k \right], \end{aligned} \quad (10)$$

where \hat{b} is the annihilation operator of the medium excitations (*e.g.* excitons or optical phonons), which we

assume here to be dispersionless having frequency ω_T ; Ω_P denotes the light-medium coupling strength that is proportional to the Rabi frequency. In the absence of the Bragg scattering term ($\Omega_B = 0$) the complete Hamiltonian (1) reduces to the conventional polaritonic Hamiltonian \mathcal{H}_{pol} , given by:

$$\begin{aligned} \mathcal{H}_{\text{pol}} &= \sum_k \omega_k \hat{a}_k^+ \hat{a}_k + \omega_T \sum_k \hat{b}_k^+ \hat{b}_k \\ &+ \Omega_P \sum_k \left[\hat{b}_k^+ \hat{a}_k + \hat{a}_k^+ \hat{b}_k \right], \end{aligned} \quad (11)$$

with eigenstates representing the mixture of light and medium excitations

$$\begin{aligned} \hat{a}_k &= \cos\psi \hat{\pi}_1(k) + \sin\psi \hat{\pi}_2(k), \\ \hat{b}_k &= -\sin\psi \hat{\pi}_1(k) + \cos\psi \hat{\pi}_2(k), \end{aligned} \quad (12)$$

where

$$\cos 2\psi = \frac{\omega_k - \omega_T}{\sqrt{(\omega_k - \omega_T)^2 + 4\Omega_P^2}}, \quad (\omega_k = ck/\sqrt{\varepsilon_0}). \quad (13)$$

With the new operators $\hat{\pi}_1$ and $\hat{\pi}_2$, the Hamiltonian (11) is diagonalized:

$$\begin{aligned} \mathcal{H}_{\text{pol}} &= \sum_k \omega_P^{(1)}(k) \hat{\pi}_1^+(k) \hat{\pi}_1(k) \\ &+ \sum_k \omega_P^{(2)}(k) \hat{\pi}_2^+(k) \hat{\pi}_2(k), \end{aligned} \quad (14)$$

where the frequencies of the polaritonic branches are given by

$$\omega_P^{(1,2)}(k) = \frac{1}{2} \left[\omega_k + \omega_T \pm \sqrt{(\omega_k - \omega_T)^2 + 4\Omega_P^2} \right]. \quad (15)$$

The Rabi splitting at resonance, *i.e.* at $\omega_k = \omega_T$ is $2\Omega_P$. Eq. (15) allows to express the phenomenological parameter Ω_P through the observables. Namely, $\Omega_P = \sqrt{\omega_T \omega_{\text{LT}}}/2$, where $\omega_{\text{LT}} \ll \omega_T$ is the transverse-longitudinal splitting.

We note that the above description is valid only for wavenumbers k in the vicinity of “crossing” of the excitation branches, where $\omega_k \simeq \omega_T$. It does not capture, however, the correct behavior¹⁸ of the polaritonic branches for $k \rightarrow 0$. In this limit an additional term of the type $a_k b_{-k} + \text{c.c.}$ should be taken into account in Eq. (11).

III. Diagonalization of the full Hamiltonian

Now let us consider the full Hamiltonian (1) with both Bragg scattering and light-medium interaction included,

$$\begin{aligned}
\mathcal{H} = & \sum_q [\omega(q)\hat{a}_{\rightarrow}^+(q)\hat{a}_{\rightarrow}(q) + \omega(-q)\hat{a}_{\leftarrow}^+(-q)\hat{a}_{\leftarrow}(-q)] \\
& + \Omega_B \sum_q [e^{i\phi} \hat{a}_{\rightarrow}^+(q)\hat{a}_{\leftarrow}(-q) + e^{-i\phi} \hat{a}_{\leftarrow}^+(-q)\hat{a}_{\rightarrow}(q)] \\
& + \omega_T \sum_q [\hat{b}_{\rightarrow}^+(q)\hat{b}_{\rightarrow}(q) + \hat{b}_{\leftarrow}^+(-q)\hat{b}_{\leftarrow}(-q)] \\
& + \Omega_P \sum_q [\hat{b}_{\rightarrow}^+(q)\hat{a}_{\rightarrow}(q) + \hat{a}_{\rightarrow}^+(q)\hat{b}_{\rightarrow}(q) \\
& + \hat{b}_{\leftarrow}^+(-q)\hat{a}_{\leftarrow}(-q) + \hat{a}_{\leftarrow}^+(-q)\hat{b}_{\leftarrow}(-q)], \quad (16)
\end{aligned}$$

where we have again truncated the “Bragg” Hamiltonian in (1) by including only near-resonance terms. If a col-

umn of operators $\hat{c} = \{\hat{a}_{\rightarrow}(q), \hat{a}_{\leftarrow}(-q), \hat{b}_{\rightarrow}(q), \hat{b}_{\leftarrow}(-q)\}$ is introduced, then the Hamiltonian (16) can be formally rewritten in a matrix form $\mathcal{H} = \hat{c}^\dagger H \hat{c}$, where

$$H = \begin{pmatrix} \omega(q) & \Omega_B e^{i\phi} & \Omega_P & 0 \\ \Omega_B e^{-i\phi} & \omega(-q) & 0 & \Omega_P \\ \Omega_P & 0 & \omega_T & 0 \\ 0 & \Omega_P & 0 & \omega_T \end{pmatrix}. \quad (17)$$

The four H eigenvalues yield the dispersion relations of the *four* excitation branches, whereas the eigenvectors determine the unitary transformation diagonalizing \mathcal{H} .

The characteristic equation for the eigenvalues ω of the matrix H reads

$$\left[(\omega(q) - \omega)(\omega(-q) - \omega) - \Omega_B^2 - \left(\frac{\omega(q) + \omega(-q) - 2\omega}{\omega_T - \omega} \right) \Omega_P^2 \right] (\omega_T - \omega)^2 + \Omega_P^4 = 0. \quad (18)$$

If the light-matter coupling is absent, *i.e.* $\Omega_P = 0$, then the roots of (18) reduce to two pure medium excitations with unperturbed frequency ω_T propagating in the forward and backward directions along z , and two purely photonic excitations with dispersion relation given by Eq. (9) that results from the Bragg scattering. If, on the other hand, the Bragg scattering is absent, *i.e.* $\Omega_B = 0$, then the roots of Eq. (18) reduce to two pairs of polariton branches with dispersion relation given by Eq. (15).

It appears that the unitary transformation in *four-dimensional* space diagonalizing the Hamiltonian \mathcal{H} can be parameterized by *two* angles:

$$\begin{pmatrix} \hat{a}_{\rightarrow}(q) \\ \hat{a}_{\leftarrow}(-q) \\ \hat{b}_{\rightarrow}(q) \\ \hat{b}_{\leftarrow}(-q) \end{pmatrix} = \begin{pmatrix} \cos\theta \cos\tilde{\psi} & \sin\theta \sin\tilde{\psi} & \cos\theta \sin\tilde{\psi} & \sin\theta \cos\tilde{\psi} \\ \sin\theta \cos\tilde{\psi} & -\cos\theta \sin\tilde{\psi} & \sin\theta \sin\tilde{\psi} & -\cos\theta \cos\tilde{\psi} \\ \cos\theta \sin\tilde{\psi} & \sin\theta \cos\tilde{\psi} & -\cos\theta \cos\tilde{\psi} & -\sin\theta \sin\tilde{\psi} \\ \sin\theta \sin\tilde{\psi} & -\cos\theta \cos\tilde{\psi} & -\sin\theta \cos\tilde{\psi} & \cos\theta \sin\tilde{\psi} \end{pmatrix} \cdot \begin{pmatrix} \hat{\mathcal{B}}_2 \\ \hat{\mathcal{I}}_2 \\ \hat{\mathcal{I}}_1 \\ \hat{\mathcal{B}}_1 \end{pmatrix}, \quad (19)$$

where $\hat{\mathcal{B}}_1$, $\hat{\mathcal{I}}_1$, $\hat{\mathcal{I}}_2$, and $\hat{\mathcal{B}}_2$ are new operators that annihilate mixed light-matter states. The angle θ in Eq. (19) is precisely the “Bragg” rotation angle introduced in Eq. (7) [for simplicity we set $\phi = 0$ for the modulation phase in Eq. (19)]. The second angle, $\tilde{\psi}$ is defined by the following relation

$$\cos 2\tilde{\psi} = \frac{\sqrt{[\omega(q) - \omega(-q)]^2 + 4\Omega_B^2} - 2(\omega_T - \omega_B)}{\sqrt{\left\{ 2(\omega_T - \omega_B) - \sqrt{[\omega(q) - \omega(-q)]^2 + 4\Omega_B^2} \right\}^2 + 16\Omega_P^2}}. \quad (20)$$

Naturally, for $\Omega_B = 0$ the angle $\tilde{\psi}$ reduces to the polaritonic rotation angle ψ in Eq. (13). In the presence of the Bragg scattering, however, this rotation angle also depends on the “Bragg” parameters ω_B and Ω_B . Therefore it is the angle $\tilde{\psi}$ that characterizes the interplay between the polaritonic and diffraction effects.

IV. Braggoritonic excitations

In order to analyze the solutions of Eq. (18), it is convenient to introduce the following dimensionless variables. We measure frequencies, Δ , from the Bragg frequency, ω_B , and express them in units of the Bragg gap $2\Omega_B$:

$$\Delta = \frac{\omega - \omega_B}{2\Omega_B}. \quad (21)$$

In analogy with Eq. (21) we introduce the dimensionless frequency detuning, δ , of ω_T from the Bragg frequency ω_B , where

$$\delta = \frac{\omega_T - \omega_B}{2\Omega_B}. \quad (22)$$

As seen from Eq. (9), the natural unit for the wavevector deviation, q , from the Bragg wavevector, $\sigma/2$, is $\sigma\Omega_B/\omega_B$. Hence, we introduce the dimensionless parameter

$$Q = \left(\frac{\omega_B}{\sigma\Omega_B} \right) q. \quad (23)$$

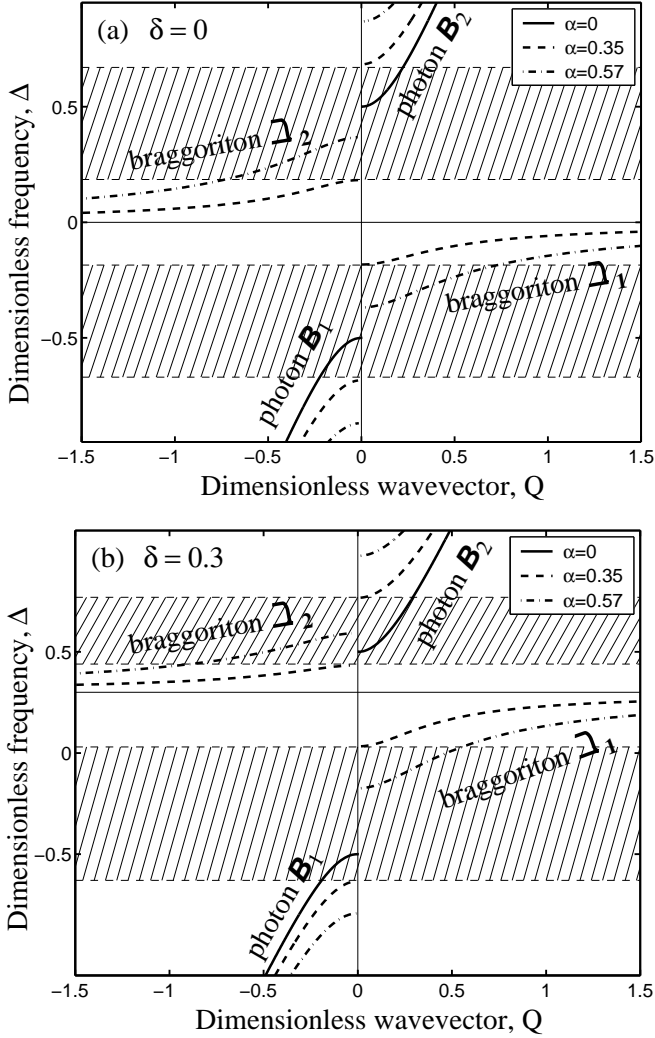


Fig. 1 Dispersion of mixed photonic-medium excitations for various coupling strengths: $\alpha = 0, 0.35, 0.57$. (a) $\delta = 0$; (b) $\delta = 0.3$. The shaded area represents the two forbidden subgaps at $\alpha = 0.35$.

With the new notations, the excitation spectrum determined by Eq. (18) can be rewritten in a more concise form

$$|Q| = \sqrt{\left(\Delta - \frac{\alpha^2}{\Delta - \delta}\right)^2 - \frac{1}{4}}, \quad (24)$$

where $\alpha = \Omega_P/(2\Omega_B)$ characterizes the relative strength of the Bragg and polaritonic couplings. Expression (24) is our main result. It clearly demonstrates that the Bragg and polaritonic dispersion relations *compete* with each other.

Consider for simplicity the case of exact resonance, *i.e.* $\delta = 0$. It is seen from Eq. (24) that in the absence of light-matter coupling ($\alpha = 0$), the first term in the brackets gives rise to the conventional PBG. It is also seen that with increasing α (or, Ω_P) the decay length, $\text{Im } Q^{-1}$, increases, and for sufficiently small Δ we find

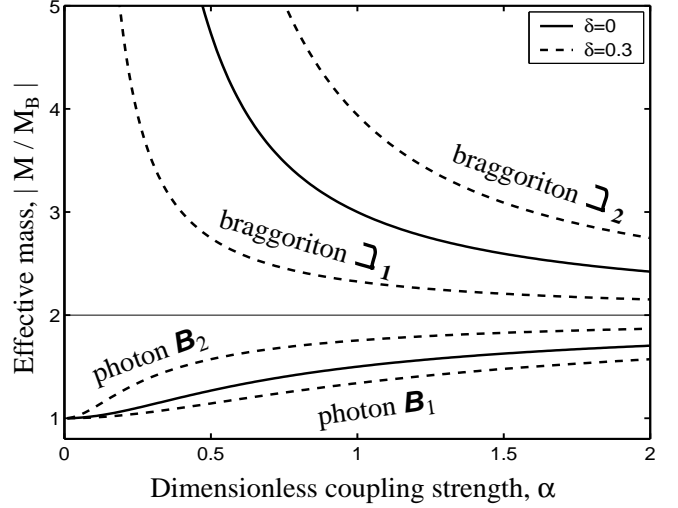


Fig. 2 The effective mass for various excitations (in units of “free” Bragg mass $M_B = M_{B_1} = M_{B_2}$ at $\alpha = 0$) is plotted vs. coupling strength: solid lines are for $\delta = 0$ where $M_{B_1} = M_{B_2}$, $M_{1_1} = M_{1_2}$; dashed lines are for $\delta = 0.3$.

that Q becomes *real*. This manifests the emergence of the novel *allowed* photonic states, or braggoritons, inside the PBG (see Fig. 1). The braggoriton branches in the excitation dispersion relations are described by the operators $\hat{\mathbf{1}}_1$ and $\hat{\mathbf{1}}_2$. They occupy the frequency ranges $\Delta = \left[0, \pm \frac{1}{4}(\sqrt{1 + 16\alpha^2} - 1)\right]$. For small α ($\alpha \ll 1$), the braggoriton frequency interval reduces to $(0, \pm 2\alpha^2)$. We note that due to the finite α value the Bragg gap broadens. Namely, the band edges of the branches described by the operators $\hat{\mathbf{B}}_1, \hat{\mathbf{B}}_2$ are respectively given for $\delta = 0$ by $\Delta = \pm \frac{1}{4}(\sqrt{1 + 16\alpha^2} + 1)$ (compare to $\Delta = \pm 1/2$ for $\alpha = 0$). The dispersion relations $\Delta(Q)$ calculated using Eq. (24) are shown in Fig. 1(a) for different values of α in the case of exact resonance $\omega_B = \omega_T$, or $\delta = 0$.

Moderate frequency detuning $\delta \neq 0$ does not qualitatively change the above picture as seen in Fig. 1(b). The major effect of frequency detuning is that the braggoritic branches $\hat{\mathbf{1}}_1, \hat{\mathbf{1}}_2$ acquire an asymmetry since they are “pinned” by ω_T . Fig. 1 also shows that the Bragg-like photonic branches $\hat{\mathbf{B}}_1, \hat{\mathbf{B}}_2$ are affected by coupling or detuning only weakly.

To quantitatively describe the braggoriton dispersion relation, we consider two characteristics: (i) dimensionless effective mass, M near the band edges that is defined from Eq. (24) by the relation,

$$\Delta \simeq \Delta_{Q=0} + \frac{Q^2}{2M}, \quad (25)$$

and (ii) the density of states, $N(\Delta)$. Expanding Eq. (24) in Q yields the following effective masses for the braggoritons

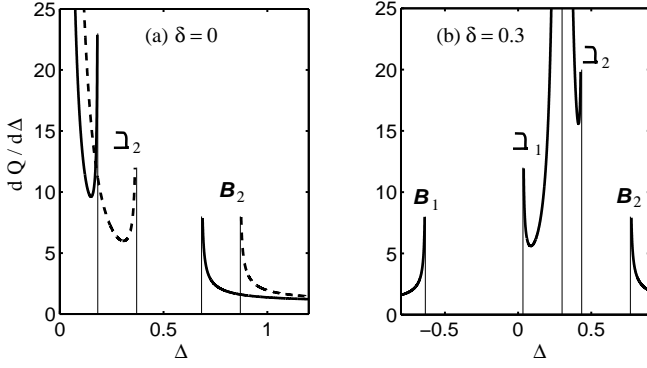


Fig. 3 Density of states for mixed photonic-medium excitations. Left panel is for the symmetric case ($\delta = 0$), for $\alpha = 0.35$ (solid line) and $\alpha = 0.57$ (dashed line). Right panel is for $\delta = 0.3$ and $\alpha = 0.35$. The thin solid vertical lines indicate the band edges.

$$M_{\mathbf{1}_1} = \left[1 - \frac{1 - 2\delta}{\sqrt{(1 - 2\delta)^2 + 16\alpha^2}} \right]^{-1}, \quad (26)$$

$$M_{\mathbf{1}_2} = - \left[1 - \frac{1 + 2\delta}{\sqrt{(1 + 2\delta)^2 + 16\alpha^2}} \right]^{-1}. \quad (27)$$

These masses are plotted in Fig. 2 versus the coupling strength α . For $\alpha \rightarrow 0$, we have $M_{\mathbf{1}_1}, M_{\mathbf{1}_2} \rightarrow \infty$, reflecting the fact that at $\alpha = 0$ the braggoritons reduce to dispersionless medium excitations that are not coupled to light. With the light-matter interaction switched on, the braggoriton effective mass rapidly decreases (the width of the in-gap branches increases).

The one-dimensional density of states $N(\Delta)$ is given from Eq. (24) by:

$$N(\Delta) \propto \frac{dQ}{d\Delta} = \frac{\Delta - \frac{\alpha^2}{\Delta - \delta}}{\sqrt{\left(\Delta - \frac{\alpha^2}{\Delta - \delta}\right)^2 - \frac{1}{4}}} \left(1 + \frac{\alpha^2}{(\Delta - \delta)^2} \right), \quad (28)$$

and shown in Fig. 3 for different values of α and detuning, δ . The density of states of the braggoritonic branches inside the gap exhibits conventional 1D square-root singularities at the band edges $\Delta = \delta$ and $\Delta = \frac{1}{2} \left[\delta \mp \frac{1}{2} \pm \sqrt{(\delta \pm \frac{1}{2})^2 + 4\alpha^2} \right]$.

As mentioned above, the upper and lower Bragg-like photonic branches, $\mathbf{B}_1, \mathbf{B}_2$, are only slightly affected by the coupling and/or detuning. In particular their effective masses,

$$M_{\mathbf{B}_1} = - \left[1 + \frac{1 + 2\delta}{\sqrt{(1 + 2\delta)^2 + 16\alpha^2}} \right]^{-1}, \quad (29)$$

$$M_{\mathbf{B}_2} = \left[1 + \frac{1 - 2\delta}{\sqrt{(1 - 2\delta)^2 + 16\alpha^2}} \right]^{-1}, \quad (30)$$

change only by a factor of 2 as α varies from zero to infinity (see Fig. 2).

V. Intragap localized states

We now turn our attention to the localized photonic states caused by a phase-slip like defect. Note that in the absence of the polarizable medium, a structure with one-dimensional modulation (3) of the dielectric function can be viewed as a distributed feedback resonator¹ first considered by Kogelnik and Shank²³ in 1972. Later it was realized that a phase slip²⁴ in the modulation

$$\varepsilon(z) = \varepsilon_0 + \delta\varepsilon \cos(\sigma z + \phi(z)), \quad (31)$$

where

$$\phi(z) = \begin{cases} \phi_1, & z < 0 \\ \phi_2, & z > 0 \end{cases}, \quad (32)$$

results in a localized state inside the PBG. Within the second quantization formalism of Sec. II, the emergence of such a state can be established as follows. Consider the eigenstate annihilation operators of the Hamiltonian (4)

$$\begin{pmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \end{pmatrix} = \begin{pmatrix} \cos \theta & -\sin \theta e^{i\phi} \\ \sin \theta e^{-i\phi} & \cos \theta \end{pmatrix} \begin{pmatrix} \hat{a}_\rightarrow \\ \hat{a}_\leftarrow \end{pmatrix}. \quad (33)$$

It follows from (33) that the absolute value, λ , of the amplitude ratio of the left and right propagating waves constituting the eigenstates β_1, β_2 is either $\lambda = \tan \theta$, or $\lambda = \tan^{-1} \theta$. These expressions are actually equivalent with appropriate choice of the sign of square root:

$$\lambda_{\pm}(\Delta) = 2 \left(\Delta \pm \sqrt{\Delta^2 - \frac{1}{4}} \right), \quad (34)$$

where we used the definition (7) of the rotation angle θ .

In the presence of a phase slip (32) the continuity condition at $z = 0$ reads

$$\lambda_-(\Delta) e^{-i\phi_2} = \lambda_*(\Delta) e^{-i\phi_1}. \quad (35)$$

As is well known²⁵ Eq. (35) has a unique in-gap solution, Δ' , for an arbitrary phase discontinuity $\phi_1 - \phi_2$,

$$\Delta' = \cos \chi, \quad (36)$$

where

$$\chi = \begin{cases} \frac{\phi_1 - \phi_2}{2} + \pi, & -\pi < \phi_1 - \phi_2 < 0, \\ \frac{\phi_1 - \phi_2}{2}, & 0 < \phi_1 - \phi_2 < \pi. \end{cases} \quad (37)$$

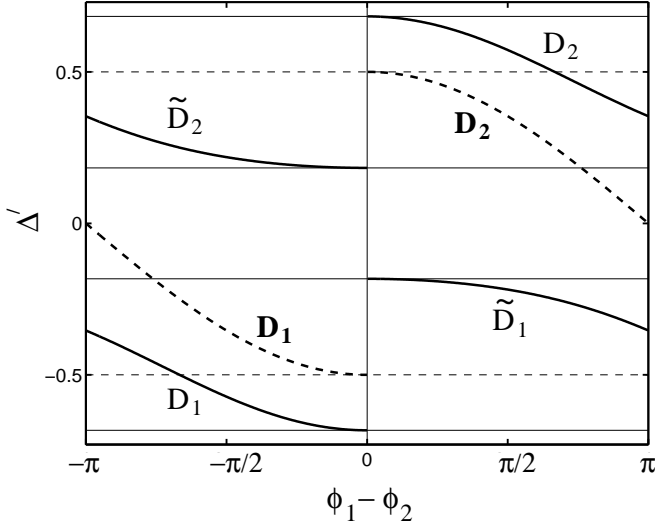


Fig. 4 The frequencies of localized intragap states vs. the phase slip magnitude: \mathbf{D}_1 , \mathbf{D}_2 are defect levels inside the Bragg gap ($\alpha = 0$, dashed line); \mathbf{D}_1 , \mathbf{D}_2 are defect levels inside the lower subgap, and \mathbf{D}_2 , \mathbf{D}_2 are defect levels inside the upper subgap ($\delta = 0$, $\alpha = 0.35$, solid line). Thin solid and dashed lines represent the band edges of the two forbidden gaps and of conventional Bragg gap (in the absence of coupling), respectively.

Generalization of the above consideration to include the polarizable medium is straightforward. It reduces to the following modification of the parameter λ in Eq. (35):

$$\lambda_{\pm}(\Delta, \alpha, \delta) = 2 \left(\Delta - \frac{\alpha^2}{\Delta - \delta} \pm \sqrt{\left(\Delta - \frac{\alpha^2}{\Delta - \delta} \right)^2 - \frac{1}{4}} \right), \quad (38)$$

Then condition (35) yields the gap state solution, Δ'

$$\Delta' = \frac{1}{2} \left[\delta + \frac{1}{2} \cos \chi \pm \sqrt{\left(\delta - \frac{1}{2} \cos \chi \right)^2 + 4\alpha^2} \right], \quad (39)$$

where χ is defined by Eq. (37). For $\alpha = 0$ we return to the in-gap state (36). Remarkably, we note that for nonzero coupling parameter α , when the Bragg gap is divided into two sub-gaps as in Fig. 1, the two values of Δ' determined by Eq. (39) are located in *each* of the corresponding sub-gaps. In Fig. 4 the frequencies, Δ' of the localized in-gap states are shown versus the magnitude $\phi_1 - \phi_2$ of the phase-slip for zero detuning $\delta = 0$.

VI. Discussion

Here we discuss the connection of the present work to the earlier related studies.

The band structure of a photonic crystal with frequency dependent dielectric function was recently studied numerically in Ref. 26, using the plane-wave method.

In this work the photonic crystal was modeled as a two-dimensional array of GaAs rods. Frequency dispersion was introduced through the transverse-longitudinal splitting of the optical phonons. The authors²⁶ (see also Ref. 27) observed that numerous branches of the band structure calculated for $\omega_B \equiv \omega_T$ become almost dispersionless at frequencies close to the frequency ω_T .

In the context of the present work, this weakening of dispersion can be understood from Eqs. (26), (27) that describes the effective masses of the braggoritonic branches $\mathbf{1}_1$, $\mathbf{1}_2$. These masses rapidly increase as the coupling parameter α decreases.

Signatures of braggoritonic excitations studied in detail in the present paper can be also found in the numerical calculations of Ref. 28. In that work, transmission spectra of a photonic crystal identical to that of Ref. 26 were calculated within the transfer-matrix formalism. *Two* minima in the transmission spectra were found instead of the usual *single* minimum that is caused by the Bragg diffraction in non-dispersive photonic crystal. In light of the theory developed in the present work, these two minima can be identified with the *two forbidden subgaps* in the excitation spectrum (Figs. 1 and 3). As we have demonstrated (Fig. 3), in the presence of light-matter coupling there are two spectral regions with zero density of states. Correspondingly, the transmission coefficient within these frequency regions must be low if the sample is sufficiently thick.

A very different realization of periodic polarizable structures was the subject of extensive theoretical studies during the last decade.^{29,30} The structures are multiple quantum wells separated by wide-gap semiconductor barriers. The width, d , of each barrier was assumed to be close to $\lambda_0/2$, where λ_0 is the wavelength corresponding to the intra-well exciton resonance frequency, ω_T . The condition $d \approx \lambda_0/2$ implies that the Bragg frequency, ω_B is close to ω_T . Since the quantum wells with strong frequency dispersion at $\omega \sim \omega_T$ had thickness much smaller than d , then a real Bragg gap in the structures^{29,30} was lacking. However, under the condition $\omega_T \equiv \omega_B$ the dispersion law of light propagating along the principal axis was shown to have a gap within a frequency range $|\omega - \omega_T| = (2\Gamma_0\omega_T/\pi)^{1/2} = \Omega^{(\text{eff})}$. Here Γ_0 denotes the radiative rate for an exciton in a single well. In other words, $\Omega^{(\text{eff})}$ plays the role of the “effective” Bragg gap in the structures.^{29,30} Remarkably, a physical picture completely analogous to the multiple-quantum-well structures emerged from consideration of an optical lattice formed by laser-cooled atoms.³¹ Correspondingly, the light dispersion relation derived in Ref. 31 has the same form as in Refs. 29, 30. In conclusion we note that as was recently pointed out³², a detuning $(\omega_B - \omega_T) \sim \Omega^{(\text{eff})}$ gives rise to a band of propagating states within the “effective” Bragg gap of the multiple-quantum-well structures.

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